

Fluopropanate-sodium
22898-01-7 | DTXSID9066837

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 9.19e-01

Global applicability domain: Inside

Local applicability domain index: 6.60e-01

Confidence level: 7.85e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl trifluoroacetate</div> <div>Measured: 1.18</div> <div>Predicted: 1.04</div>	<div>Image not found</div> <div>Acetic acid, difluoro-, ethyl ester</div> <div>Measured: 0.87</div> <div>Predicted: 8.28e-01</div>	<div>Image not found</div> <div>Acetic acid, trifluoro-, methyl ester</div> <div>Measured: 0.6</div> <div>Predicted: 7.19e-01</div>
<div>Image not found</div> <div>1-Propanol, 2,2,3,3,3-pentafluoro-</div> <div>Measured: 1.23</div> <div>Predicted: 1.14</div>	<div>Image not found</div> <div>1-Methoxy-2-propyl acetate</div> <div>Measured: 0.56</div> <div>Predicted: 4.87e-01</div>	